Gaussian 09 Revision E.01 Release Notes

14 December 2015

Contents

*Feature and Usage notes: Rev E.01

This revision is primarily to fix a variety of bugs reported by users or which were uncovered by the example jobs for the 3rd edition of *Exploring Chemistry with Electronic Structure Methods*.

♦ Formatted checkpoint files now include the version of G09 used and also a job status flag, so that GUIs can determine whether a job is still running, failed or completed successfully. The number of imaginary frequencies is also included for frequency jobs.

♦ **EOMCC=ListWindow** now reads the window only once instead of twice.

♦ Rigid (unrelaxed) scans with large energies now generate a table of relative energies rather than ****'s.

♦ The TDHF excited states method now defaults to using the MO basis, the same default as for CIS.

♦ A fix for the reference atoms used in Hirshfeld charges will change the reported charges slightly.

♦ The overhead in using Linda parallelism with ECPs was removed.

♦ The build procedures include compiling natively for Sandybridge (AVX) x86_64 processors, including an AVX-enabled ATLAS library. A Sandybridge/Haswell binary distribution is also available.

♦ The divide-and-conquer diagonalization and SVD routines work in a larger fraction of cases.

Feature and Usage Notes: Rev D.01

♦ The capabilities of the **Freq=Anharmonic** methods have been substantially expanded:

❖ Full anharmonic IR intensities are now computed [Bloino12].

❖ The DCPT2 [Kuhler96, Bloino12a] and HDCPT2 [Bloino12a] methods now support resonance-free computations of anharmonic frequencies and partition functions.

❖ Vibronic computations now include ECD [Barone12]. This code has also been significantly optimized.

❖ The output has been made more readable.

♦ Raman and ROA intensities can be calculated separately from calculation of the force constants and normal modes, to facilitate using a larger basis for these properties as recommended in [Cheeseman11a]. The keyword **Polar=Raman** (or **Polar=ROA**) requests that the force constants be picked up from the checkpoint file (i.e., from a previous **Freq** calculation) and new

polarizability derivatives (and the other two tensor derivatives for ROA) be computed and combined with the force constants in predicting intensities and spectra. Test job 931 provides an example of a two-step ROA calculation.

♦ Time-dependent DFT calculations can employ the Tamm-Dancoff approximation, via the **TDA** keyword.

♦ An energy range can be specified for CIS and TD excitation energies via the following new options to **CIS**, **TD** and **TDA**:

GOccSt=N Generate initial guesses using only active occupied orbitals N and higher.

GOccEnd=N Generate initial guesses: if $N>0$, use only the first N active occupied orbitals; if $N<0$, do not use the highest $|N|$ occupieds.

GDEMin=N Generate guesses having estimated excitation energies $\geq N/1000$ eV.

DEMin=N Converge only states having excitation energy $\geq N/1000$ eV; if $N=-2$, read threshold from input; if $N<-2$, set the threshold to $|N|/1000$ Hartrees.

IFact=N Specify factor by which the number of states updated during initial iterations is increased.

WhenReduce=M Reduce to the desired number of states after iteration M.

The default for **IFact** is $Max(4,g)$ where g is the order of the Abelian point group. The default for **WhenReduce** is 1 for TD and 2 for TDA and CIS. Larger values may be needed if there are many states in the range of interest.

♦ Several new DFT functionals and two new empirical dispersion models have been added:

❖ **EmpiricalDispersion=PFD**, **GD3** or **GD3BJ** explicitly request Petersson-Frisch dispersion [Austin12] or Grimme's D3 dispersion [Grimme10] or D3BJ dispersion [Grimme11].

❖ **APFD** requests the Austin-Frisch-Petersson functional, with dispersion [Austin12], and **APF** requests the same functional without dispersion.

❖ **B97D3** and **B2PLYPD3** request these functionals plus Grimme's D3BJ dispersion.

❖ **HISSbPBE** requests the HISS functional [Henderson08].

❖ **SOGGA11** [Peverati11], **M11** [Peverati11a], **SOGGA11X** [Peverati11b], **M11L** [Peverati12], **MN12L** [Peverat12c], **N12** [Peverati12b], **N12SX** [Peverati12a] and **MN12SX** [Peverati12a] request recent functionals from the Truhlar group.

♦ There are several options for augmenting the **cc-pV*Z** basis sets with diffuse functions:

❖ **spAug-cc-pV*Z** augments with s and p functions only, including s functions on H and He.

❖ **dAug-cc-pV*Z** augments with 2 shells of each angular momentum instead of one.

❖ Truhlar's "calendar" basis set variations [Papajak11] are available. The naming of this series of basis sets come from the fact that the cc-pV*Z basis sets with added polarization functions are known as the **Aug-cc-pV*Z**. Truhlar noted that "Aug" is also an abbreviation for the month of August in English, so he proposed new augmentation schemes for the **cc-pV*Z** basis sets, also named after months of the year. They are constructed by removing diffuse functions from the **Aug** basis sets. For example, the **Jul-cc-pV*Z** basis sets remove the diffuse function from H and He from **Aug-cc-pV*Z**. Jun-cc-pV*Z also removes the highest angular momentum diffuse function from all other atoms, **May-cc-pV*Z** removes the two highest angular momentum functions, and **Apr-cc-pV*Z** removes the three highest angular momentum functions.

Nevertheless, by default, at least s and p diffuse functions are always included in these basis sets. This serves to avoid some inherent inconsistencies, but it differs from Truhlar and coworkers' original definitions. Use the forms **TJul**, **TJun**, and so on to specify the original versions where the limit is applied unconditionally: e.g., **TMay-cc-pVDZ** includes only a diffuse s function on Cl but both diffuse s and p functions on Fe and Br, while **May-cc-pVDZ** has diffuse s and p functions on all of these atoms.

♦ Additional preliminary analysis is done on the input for MM and ONIOM(MO:MM) calculations. The moments of the charge distribution given by the MM charges are reported. If PDB information was included in the input, the net MM charges on residues are reported, as is the net MM charge in each ONIOM layer.

♦ New SCF options and features:

❖ **SCF=Big** turns off optional $O(N^3)$ steps to speed up very large calculations (>5000 basis function).

❖ **SCF=Restart** skips steps which are not necessary when restarting an SCF calculation, but which are necessary when reading in a guess from a calculation with a different basis set or at a different geometry. In contrast, if you want to start a new SCF using the restart information from a calculation with a different geometry and/or a different basis set, use **Guess=Restart**.

❖ **SCF=YQC** provides a new algorithm which is useful for difficult SCF convergence cases involving very large molecules. It does steepest descent and then scaled steepest descent as in **SCF=QC**, but then switches to regular SCF instead of quadratic convergence, using the quadratic algorithm only if the regular SCF fails to converge.

❖ **SCF=MaxNR=**N sets the threshold for switching to quadratic convergence in **SCF=QC** and to regular SCF in **SCF=YQC** to 10^{-N}. The default is 10^{-2}.

❖ Conventional SCF now works for arbitrary angular momentum. This is primarily useful with the new interface to external programs. The default of direct SCF is still preferable for calculations within Gaussian 09.

♦ There is a new, larger pruned grid, specified by **Int=SuperFineGrid**. This is about 3x larger than **UltraFine** and useful when very high accuracy is desired. The grid specification is (150,974) for the first two rows of the periodic table and (225,974) for later elements.

♦ Atomic charges:

❖ CM5 atomic charges [Marenich12] are now computed along with Hirshfeld charges. Either **Pop=Hirshfeld** or **Pop=CM5** causes both to be computed.

❖ Computed atomic charges can be stored on the checkpoint file for use in a later MM calculation with **Geom=Check**. The options **Pop=SaveMulliken**, **Pop=SaveESP**, **Pop=SaveNPA**, **Pop=SaveCM5**, and so on can be used to save the corresponding charges. In the case of a multilayer ONIOM calculation, only explicitly computed charges are saved by default: i.e., charges for atoms in the QM layer(s). Any atomic charges present in the input file will not be used and they will be replaced by the newly fitted charges saved by these options.

The additional option **Uncharged** will keep the atomic charges present in the input file and only fit charges on uncharged atoms in the QM layers(s). The option combinations **Pop=(Uncharged, SaveMulliken)**, **Pop=(Uncharged, SaveCM5)** and so on will save both the original atomic charges plus the newly fitted charges for the atoms that were originally uncharged.

❖ QEq charges are now computed using the new version of QEq [Rappe07]. **OldQEq** requests the older version which was the default in Revision C [Rappe91]. **QEq=Uncharged** now correctly sets the charges only for atoms which have MM charge zero, constraining the other atoms to retain their specified charges.

♦ An interface to NBO version 6 is provided. **Pop=NPA6**, **Pop=NBO6**, **Pop=NBO6Read** and **Pop=NBO6Delete** request use of the separate NBO6 program via the external interface. The script required to run NBO6 and the program itself must be obtained from Frank Weinhold (*nbo6.chem.wisc.edu*).

♦ **Freq=NoPrintNM** can be used to suppress printing of the normal mode components during a frequency calculation. The frequencies and intensities are still reported for each mode.

♦ The **External** command, which is used to run other programs from within Gaussian 09, has been greatly generalized. It is now possible to provide one-electron or one- and two-electron integrals and other matrix elements to an external program and to recover results such as MOs or densities from the other program. Full details and examples are in the **g09/doc** subdirectory (**doc** folder on Windows). The new options to the **External** keyword (which *must* follow the name of the script) are:

InUnf	A Fortran unformatted file will be provided to the external program containing coordinates and one-electron matrix elements (overlap, core Hamiltonian, etc.). Refer to **g09/doc/unfdat.txt** for details on the contents of the file and to **g09/doc/rdmat.F** for a sample program which reads the file and prints its contents. **1Elintegrals** is a synonym for this option.
2ElIntegtrals	The Fortran unformatted file should also contain two electron integrals. This option implies **SCF=Conventional**.
InputFchk	A formatted checkpoint file should be generated and provided to the external program.
OutputUnf	A Fortran unformatted file will be provided to the external program and an updated or replaced file with the same structure will be read by G09 for the results, in lieu of the default text output file expected from the external program/script.

IOFchk   A formatted checkpoint file will be generated and provided to the external program, and an new **.fchk** file will be read to import results afterwards.

ReadInputSection   This option can be used to alter the content of the external text input file that Gaussian 09 automatically generates for the external script. When the data transfer between Gaussian 09 and the external script is handled using one of the options above (e.g. **IOFchk**), the default external text input file is not needed. With this option, a section (delimited by the usual blank lines) will be read from the Gaussian 09 input file. The text in this section will be placed in the external text input file instead of the usual content of such file. This provides additional flexibility to provide extra instructions to the external script.

Test job 769 serves as an example of these options.

♦ The data files required by several third-party programs can be generated:

❖ **SCRF=COSMORS** produces the data file used by COSMO/RS and other programs.

❖ The data file for Antechamber (the AMBER program for generating RESP charges) can be generated using **Pop=MK IOp(6/50=1)**.

❖ The data file for the ACID program (R. Herges and D. Geuenich, *J. Phys. Chem. A* **105** (2001) 3214) can be generated with **NMR=CSGT IOp(10/93=1)**.

♦ New **Default.Route** directives:

-U-   Default memory to use in utilities such as **formchk** and **freqchk**.

-F-   Default file type argument to **formchk**.

-M-   Default amount of memory (equivalent to **%Mem**).

-L-   Default options for Linda (passed to the **GAUSS_LFLAGS** environment variable).

-R-   A synonym for **-#-**.

All of these items can also be set via environment variables or UNIX command line arguments. The environment variable **GAUSS_XDEF** provides a line equivalent to -*X*- in the **Default.Route** file. Similarly, the command line argument to **g09** -*x*=**"value"** specifies the same setting. For example, all of the following have the equivalent effect:

-M- 4GB in Default.Route
export GAUSS_MDEF=4GB
g09 -m="4GB" ...

The order of priority is: command line argument, environment variable, **Default.Route** setting, internal program default.

♦ **Geom=NGeom=***N* retrieves the *N*th geometry from an optimization checkpoint file using the same record of points used for display in GaussView, where *N*=1 corresponds to the input molecule specification. **Geom=Step=***M* is automatically converted to **Geom=NGeom=***M*+1 if the previous optimization used redundant internal coordinates.

♦ A bond order of **0.1** can be specified in **Geom=Connectivity** input to specify a bond which should be used in generating internal coordinates but which should not affect atom types or connectivity for molecular mechanics.

♦ New Link0 Directives:

%UseSSH   Start Linda workers using **ssh** rather than **rsh**.

%DebugLinda   Report details concerning the starting and stopping of Linda workers.

♦ The ECP potential name **def2** or the synonym **QZV** can be used in **GenECP** input to request the potentials which are used with both the def2 and QZV basis sets.

♦ Generation of various types of internal coordinates can be suppressed:

Geom=SkipAll   Suppresses automatic generation of any internal coordinates; all of them must be explicitly specified in the **Geom=ModRedundant** input section.

Geom=SkipAng   Generates bonds but omits angles and dihedrals.

Geom=SkipDihedral   Suppresses the generation of dihedrals.

Geom=SkipHBond   Skips generation of hydrogen-bond coordinates.

- **IRC=GradientOnly** now defaults to **EulerPC** rather than **DVV**. Analytic second derivatives can be done intermittently during IRCs using **IRC=(CalcFC,RecalcFC=(Predictor=**N**,Corrector=**M**))** which computes second derivatives at the initial point and then at every Nth predictor step and every Mth corrector step.

- Performance improvements:

  - CIS and TD calculations now use symmetry more effectively.

  - Calculations using two electron integrals stored in memory now use integrals over symmetry-adapted basis functions, speeding up calculations when symmetry is present and reducing the memory required for in-core calculations on open-shell systems.

  - The option **Force=NoStep** can be used with large MM force calculations to avoid the $O(N^3)$ work involved in computing the putative geometry optimization step.

- Minor changes to input and input handling:

  - The handling of **DFTB** input files has been modified for compatibility with the files provided by Elstner: HTML data at the end of the file is now ignored. Also, multipliers--e.g., **10*1.0**--are now accepted. However, some modifications to Elstner's files are still required for use with G09; see *http://www.gaussian.com/g_tech/g_ur/k_dftb.htm#dftbinput* for details.

  - The extension used for scratch file, which was **.scr**, is now **.skr**. This change was made to avoid problems with Windows virus detection software.

  - The UNIX and Mac OS X versions of the program now look for an input file with extension **.gjf** first when no extension is specified. If not **.gjf** file is found, a file with extension **.com** will be looked for next.

  - Specifying an initial value for a defined coordinate is no longer supported in **Opt=ModRedundant** input. Instead, the input structure should be modified to reflect the desired initial value and the input value omitted from the coordinate definition.

  - Optional additional input for **Freq=AnHarmonic** has changed format. See the section "Additional Input for **Freq=ReadAnHarmon**" in the online version of the **Frequency** keyword documentation: *http://www.gaussian.com/g_tech/g_ur/k_freq.htm#AnharmInput*.

Feature and Usage Notes: Rev C

- Changes to optimization algorithms and options:

  - The selection of modes to include when stepping down from a region of wrong curvature during an optimization has been improved. This can also now be controlled by route options:

Opt=NoDownHill	Don't try to go downhill; just take an RFO-like step.
Opt=NGoDown=m	Mix at most m eigenvectors in taking a downhill step. The default is 3.

  - Linear bends are handled more reliably, and included in internal coordinate more frequently, than before. This avoids many optimization problems involving nearly linear angles becoming exactly linear.

  - The connectivities of reactant and product are now merged in generating the internal coordinates for the TS during QST2 and QST3 optimizations.

  - The maximum number of steps allowed ever in an optimization (i.e., include later restarts) can be reduced. This is sometimes useful for very large systems in order to reduce memory and disk usage.

  - The program now checks if the standard orientation of a molecule has flipped by 180 degrees during an optimization and avoids the flip. This avoids jumps when animating optimizations, IRCs, etc. in GaussView and improves SCF convergence.

  - The memory allocation for generation of internal coordinates is now proportional to the amount of memory provided by **%Mem**. This allows jobs with very large numbers of atoms or internal coordinates which previously failed to run if enough memory is provided.

  - By default, internal coordinates for potential hydrogen bonds are not generated automatically. Bond coordinates are still added to connect otherwise disjoint fragments, so coordinates for hydrogen bonds which connect fragments will still be included.

- Single-point BD calculations now default to frozen-core, with the core orbitals uncorrelated but updated using the BD Fock matrix. The previous default was to leave the core orbitals unchanged from the HF values, or from the orbitals read in with **BD=Read**. The new default produces energies which are independent of the choice of starting orbitals. Gradients with BD still require and defaults to full rather than frozen-core. The **OldFCBD** keyword requests the old-style frozen-core.

- On some machines fully direct integral transformation and fully direct MP2 are chosen if there is a large amount of memory, but the semi-direct algorithms are faster. **Tran=SemiDirect** in the **Default.Route** file now forces the semi-direct algorithm for MP2 as well as the transformation in higher level post-SCF calculations. Note that all method keywords such as **MP2** are ignored in the **Default.Route** file, because otherwise they would force that model in all calculations.

- **Output=Wfn** and **Output=WfX** with post-SCF methods now default to **Density=Current** and **Pop=NOAB**, both of which are necessary for the post-SCF density to be stored in the **.wfn/.wfx** file. Problems with the orientation of the forces in these files and in generating them with ROHF wavefunctions and/or linearly dependent basis sets have also been fixed.

- Several customers have used the file generated for COSMORS as input to their local simulation programs, so this capability has been put back into G09.

- **Polar=Gamma** has been added as more descriptive option for requesting second hyperpolarizabilities. It is synonym for **Polar=(DCSHG,Cubic)**.

- The **RevTPSS** exchange and correlation functionals have been added.

- **SDD** now defaults to more recent basis sets for actinides; **OldSDD** requests the previous default.

- **TB** and **TW** can now be used to specify memory and disk allocations in units of terabytes and terawords, respectively.

- The **Direct** option is available for SAC-CI. This requests an integral-direct algorithm suitable for larger molecules.

- A **%OldChk** Link0 command has been added. The contents of the checkpoint file specified by **%OldChk** are copied to the checkpoint file of the current job step at the start of the job step. This allows data to be picked up from a previous calculation without destroying anything on the checkpoint file from it.

- Diffuse (**aug-**) functions were added for **cc-pVDZ** for the first transition row.

- A Windows64 version is now available.

Feature and Usage Notes: Rev B

- NewZMat now writes out secondary structure information, if present, with **-opdb**.

- NewZMat can now merge data from two input files. Either two text files or an input and a checkpoint file can be merged.

- **Polar=(Cubic,DCSHG)** can now be used to numerically differentiate frequency-dependent hyperpolarizabilities (betas) to produce second hyperpolarizabilities (gammas). These polarizabilities are now printed in the standard coordinate systems (i.e., with components of beta along and perpendicular to the dipole moment).

- WfnX files, used by the newer versions of AIMPAC, can now be written via **Output=WfnX**.

- Performance for very large MM systems (>20K atoms) has been improved, especially when range limits are applied to the Coulomb and Van der Waals terms. There is a new route option, **Geom=Huge**, which turns off various actions, useful in QM calculations but unnecessary and expensive with enormous MM runs.

- **MaxDisk** can now be specified in the **Default.Route** file.

- The Hu, Lu and Wang charge fitting model [Hu07] is now available via **Pop=HLY**. The authors only parametrized the atomic densities required for the model for the first 18 elements. An alternative version, **Pop=HLYGAt**, uses the HLY fitting scheme but with Gaussian's standard atomic densities, which are available for the entire periodic table. For systems which can be done either way, the difference in atomic charges is usually between 1% and 5%.

- The SCVS method of Todd Keith, which scales the molecule in order to make the virial condition satisfied exactly, has been added.

Feature and Usage Notes: Rev A

♦ If CIS frequencies are to be used with the Herzberg-Teller or Franck-Condon-Herzberg-Teller analysis, the CIS frequencies must be done numerically (**Freq=Numer** rather than **Freq**). This is because the transition dipole derivatives are not computed during the analytic force constant evaluation. The corresponding HF frequency calculation on the ground state, which is also required, can be done analytically as usual.

♦ CIS and CASSCF frequencies with PCM solvation must also be done numerically using **Freq=Numer**.

♦ The linear scaling (FMM-based) algorithms are now Linda-parallel, so Linda parallel jobs on large molecules do not need to specify **NoFMM**, and will run faster with the default algorithms chosen by the program.

♦ **Opt=GDIIS** is still present but deprecated; the new default optimization algorithm (**Opt=GEDIIS**) is better than GDIIS for the few cases where GDIIS was better than the G03 default (**Opt=RFO**).

♦ Optimizations of large molecules which have many very low frequency vibrational modes with DFT will often proceed more reliably when a larger DFT integration grid is requested (**Int=UltraFine**).

♦ Density fitting can be made the default for jobs using pure DFT functionals by adding the **DenFit** keyword to the route section (−#−) line in the **Default.Route** file. Fitting is faster than doing the Coulomb term exactly for systems up to several hundred atoms (depending on basis set), but is slower than exact Coulomb using linear scaling techniques (which are turned on automatically with exact Coulomb) for very large systems.

♦ The default IRC algorithm has changed; refer to the *Users Guide* for details. The default is to report only the energies and reaction coordinate at each point on the path; if geometrical parameters along the path are desired, these should be defined as redundant internal coordinates via **Geom=ModRedundant** or as input to the IRC code via **IRC(Report=Read)**.

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Zhao06c	Y. Zhao and D. G. Truhlar, "Density Functional for Spectroscopy: No Long-Range Self-Interaction Error, Good Performance for Rydberg and Charge-Transfer States, and Better Performance on Average than B3LYP for Ground States," *J. Phys. Chem. A* **110** (2006) 13126-30.

Citation Corrections

The references for variations of the M06 functional were swapped and incomplete. The correct references are: M06HF [Zhao06b,Zhao06c], M062X [Zhao08]. The M05 functionals are also still available: M05 [Zhao05] and M052X [Zhao06].

Errata to the Printed Gaussian 09 User's Reference

♦ The following are missing from the list of links (pp. 38-39):

L117 Performs IPCM calculations.
L610 Numerical integration (for testing integral codes).

- The following links included in the list are not part of Gaussian 09: L909, L921, L922.

- The "Thresh" keyword described in the discussion of selecting normal mode output on pages 107 and 289 is not available.

- The reference to **Opt=DiagFull** on page 116 should be **Freq=DiagFull**.

Errata to the Printed Gaussian 09 IOps Reference
The description of IOps(1/111-113) is incorrect. Here is the corrected version:

IOp(1/111)
L103: Step-size to use with steepest descent when L103 is having trouble.

-N	Scale up to RMS step of N/1000 if DXRMS is less.
-1	Effectively disables the scaling.
0	Default (50).
N	Scale up or down to maximum change in a variable of N/1000.

L101: Temperature for thermochemistry.

0	Default (standard temperature, unless read in).
N	N/1000 degrees.
-N	N/1000000 degrees.

IOp(1/112)
Pressure for thermochemistry.

0	Default (1 atmosphere, unless read in).
N	N/1000 atmospheres.
-N	N/1000000 atmospheres.

IOp(1/113)
Scale factor for harmonic frequencies for use in thermochemistry and harmonic vibration-rotation analysis.

0	Default (1 unless specified by IOp in overlay 7 or read in).
N	N/1000000.

- Note that IOp(1/114) is not defined.

Building from Source Code

- Building Gaussian 09 with Linda requires Linda version 8.2; the executables will not build with previous version of Linda.

- Building on Intel Macs requires a case-sensitive file system.

- In order to build the 32-bit version on Mac OS X systems, you must specify:

    $ **bsd/bldg09 all mac32**

  The default is to build for 64-bit systems.

- In order to build the Power 5 or Power 6 version on the relevant IBM systems, you must specify:

    $ **bsd/bldg09 all ibmp**n

  where n is **5** or **6**. The default is to build the Power 7 version under both Linux and AIX.

Corrections to Deprecated Features:

- Problems with setting non-integer nuclear charges in **Massage** input have been corrected. There is now a **ZNuc** function in **Massage** input which changes the nuclear charge but not the atomic number.

*Bug fixes between Gaussian 09 Revisions E.01 and D.01:

- A problem in computing gradients with Bruckner Doubles with a linearly dependent basis set was fixed.

- Certain basis sets produced an error at the beginning of the frequency step of an **Opt Freq** compound job. This has been fixed.

- Problems with the NBO (version 3) included with Gaussian with some ECPs were fixed.

- A problem which occurred when a closed-shell optimization had a decrease in the number of linearly dependent basis functions during a step in which the energy went up was fixed.

- A problem in doing **Stable=Opt** with **SCF=XQC** was fixed.

- A problem using the **unfchk** utility on an **.fchk** files from an RO calculation was fixed.

- There were fixes to printing and reading of the "DCore" parameters for semiempirical methods such as AM1 and PM6.

- Several problems in generating the route for the frequency part of an **Opt Freq** compound job were fixed:
  - An inconsistency when using a density functional which included either the **PBEHl** or **wPBE** exchange functionals.
  - **DFT TDA Opt Freq** compound jobs failed, producing a garbage route.

- A bug in computing CM5 charges was fixed

- A bug in how user-provided non-standard parameters for water in the SMD solvation model was fixed.

- A problem in printing normal mode electric field derivatives when extra print was requested was fixed.

- **CIS=50-50** and **TD=50-50** calculations no longer repot erroneous non-zero transition dipole vectors between states of different symmetries.

- A missing factor of 1/2 in ECP spin-orbit integrals was added. ECP calculations which do not request spin-orbit were correct, and all-electron DKH calculations which include spin-orbit were also correct.

- A problem with specifying non-integer nuclear charges in **Massage** input was fixed.

- Magnetic susceptibilities when FMM was in use were corrected.

- A problem with **NMR=Mixed** when ECPs were in use was fixed.

- An erroneous error message for **O3LYP** was removed.

- Errors which produced garbage energies for Douglas-Kroll-Hess calculations using a completely uncontracted basis set were fixed.

- The keyword combination **MP2 NMR=Mixed** now generates an error rather than a nonsense route.

- **ADMP=Restart** for open-shell systems now works.

- Some dimensioning problems for **CAS** with more than 255 basis functions were fixed.

- **Opt=MaxCyc=**N now works correctly when N was larger than the default limit of 6 x number-of-atoms.

- Iterative Hirsheld charges now function correctly.

- Frequencies using **GD3BJ** dispersion are now correct. Frequencies for other variants of Grimme D3 dispersion were correct in D.01 unless atoms having coordination numbers of 8 or more were involved.

- **TDA Freq** now generates a correct route.

Bug Fixes between Gaussian 09 Revisions D.01 and C.01:

- A bug in the setup of basis sets for **DFTB** for Cu and Zn atoms was fixed.

- Problems generating **.wfx** files for post-SCF methods was fixed. Various other bugs with respect to these files were also corrected.

- Calculations with the **QZVP** basis and heavy atoms now set up and use the corresponding ECPs correctly.

- The input for angular momentum shells larger than k are now parsed correctly through L=13, and a problem with evaluation of integrals with L=10 and higher is fixed. Also note that Gaussian assigns the shell for L=7 as j.

- The **cubegen** utility now correctly produces Laplacian and ROHF density. It also now correctly computes the current density from jobs with basis sets with pure functions (5d 7f).

- The **Freq=DoTemp** feature is now implemented.

- Two bugs in the **50-50** option for excited state calculations have been fixed.

- Bug in the **Pop=SaveNTO** option has been fixed (it is not longer necessary to add **IOp(6/22=-14)**).

- A change in the format of the output caused problems for GaussView 5 when reading Gaussian 09 C.01 output files with modified redundant internal coordinates and ONIOM jobs. This has been fixed.

- A bug in the report of the entropy in **Freq=Anharmonic** output for saddle points (one or more imaginary frequencies) has been fixed.

- A memory bug specific to G09 Rev. C.01 for 64-bit Windows in post-SCF jobs has been fixed.

- A bug that affects the **Opt=QST2** and **Opt=QST3** with frozen atoms has been fixed.

- A bug in the combination of a ESP charge fitting scheme (e.g. **Pop=MK**) and the report of electrostatic properties at a list of points given in the input (**Prop=Read**) has been fixed.

- A bug has been fixed where the initial energy for the linear search in **SCF=QC**, **SCF=SD** and **SCF=SSD** procedures was being set incorrectly, which occasionally would caused the linear search to stop because it was unable to find a lower energy.

- A bug reading the **ECP** section in ONIOM jobs has been fixed. When using atomic symbols to select atoms to which the ECP should be applied and the first atom with that element symbol is in the MM layer, the ECP was not applied to any other atom with the same element symbol.

- A bug in **formchk** for restricted open shell cases (RO) has been fixed; the total density and the spin density are now correctly saved in the formatted checkpoint file.

Bug Fixes and Minor Changes between Gaussian 09 Revisions C.01 and B.01:

- The memory required by very large ONIOM(MO:MM) and pure MM frequency calculations has been reduced.

- The definition of improper torsions in the Amber force field is dependent on the ordering of atoms in the molecule. Calculations in the Amber program on typical proteins are consistent because of the standard ordering of atoms within residues and residues within a PDB file, but for general molecules produced with GaussView the results depend on the order of atoms in an arbitrary way. G09 has been changed to average over the 6 possible orders of atoms in an Amber improper torsion, making the results slightly different than the standard Amber force field, but making the energy independent of permutations of atoms in the molecule.

- Printing during **Pop=MK** with **IOp33** increased has been restored to include the data required for RESP charge fitting. However, G09 can now generate the data file for AnteChamber directly, by setting **IOp(6/50=1)** in the **Pop=MK** job, and this is the recommended method for generating input for RESP.

- A bug in CIS frequencies with PCM solvation was fixed.

- **MaxDisk** in a **Default.Route** file now applies to all steps of a compound job; previously, only the first step was defaulted properly.

- A bug which prevented reading AlpB parameters for AM1 was fixed.

- Convergence during SCVS calculations is now checked more carefully.

- **Pop=SaveBio** in **Stable=Opt** jobs caused the stability calculation to be wrong or fail. This now works properly, saving the biorthogonal orbitals only after the wavefunction has been made stable.

- External point charges now work with symmetry turned on.

- A bug in TD-DFT gradients with frozen core was fixed.

- Print statements for NMR shielding were fixed to work with more than 999 atoms.

- A bug in DFTB using interpolated (not analytic) parameters with d functions was fixed.

- A rare problem with uncompleted write statements on slow file systems was fixed.

- Problems with some combinations of charge and multiplicity in fragments during **Guess=Fragment** calculations were fixed.

- Printing of Coriolis terms during **Freq=VibRot** was restored.

- Some memory allocation problems for PBC calculations with large unit cells were fixed.

- Inconsistencies in how the geometry was modified in some cases by **Symm=Loose** were fixed.

- A bug in the ROMP4 triples energy when **NoSymm** was specified was fixed.

- An ominous sounding but unnecessary warning from the CBS extrapolation was turned off.

- ONIOM(MO:MM) jobs which do microiterations and which fail to finish are now restartable.

- A bug in reading ECPs with ONIOM when the same ECP was placed on multiple centers was fixed.

- The combination of **IRC** and **Freq**, which did the frequency calculation at the last point of the IRC rather than the TS, is now rejected.

- Several unsupported combinations of Douglas-Kroll-Hess with properties now generate an error message rather than incorrect answers.

- A bug in generating the default (Harris) initial guess when using ECPs on charged species was fixed. The quality of the initial guess when using ECPs has also been improved.

- Several defaults for whether to use FMM and other integral options have been updated for better performance on current models of CPU.

- **Formchk** now writes -1 rather than ****** to the formatted checkpoint file if the value exceeds 10^{13}-1. This allows **unfchk** and other utilities to process the resulting .**fchk** file.

- A bug affecting **Geom=Check** after numerical frequencies when using ONIOM was fixed.

- The combination of **BD** or **W1BD** with **SCRF**, which does not work correctly, is now rejected by the route generator.

- A new version of the ATLAS BLAS library is used on most platforms. This fixes several problems when using very large amounts of memory. However, in the event of any lingering problems of this type, **IOp1=NoAssem** can now be specified on the route line to turn of use of the ATLAS matrix multiplication routines.

- A problem in reported transition moments between excited states computed in SAC-CI jobs was fixed.

- Empirical dispersion with DFT and ghost atoms now runs. Empirical dispersion and PBC now produced an error message, since it is not implemented.

- **Opt Freq** with **ROHF/RODFT** now works correctly, doing **Freq=Numer** with the restricted open-shell wavefunction in the second job step.

- Franck-Condon calculations now function correctly for forbidden transitions.

- The route generator rejects the combination of **TD** and double-hybrid DFT methods, which never worked (previously, TD was done based on only the SCF part of the double-hybrid).

- **IRC=(RCFRC,GradientOnly)** calculations now correctly use the Hessian from the checkpoint file.

- A memory allocation bug for very large systems, which could cause a failure with the message "NIJ > Max2 in MMCore," was fixed.

- The **External** keyword functions correctly in the Windows version. Consult **g09\tests\com\test726.gjf** for an example of using it.

- A problem with the G09W front-end writing out multi-step jobs when the **--Link1--** lines were truncated was fixed.

Bug Fixes and Minor Changes between Gaussian 09 Revisions B.01 and A.02:

- A bug in MP2 frequencies with PCM was fixed.

- An updated version of the SAC-CI code is included. This includes a new integral-direct algorithm, specified with **SACCI=(Direct, …)** , which is much faster for large systems.

- The **ExtraOverlay** route keyword did not function in Revision A.02; this has been corrected.

- **Opt Freq TD** calculations now run both job steps properly.

- Problems with the dummy basis set used with Molecular Mechanics for systems that are highly charged or have very high spin were fixed.

- The free-format input routines have been generalized in order to make data from newer DFTB parameter files acceptable. These files still require some modification to be used with G09.

- The full tensors for ECD using TDDFT (including the quadrupole component) are now printed.

- The use of IOps to specify user-selected ranges for integrals has been updated in order to make it more general.

- The default algorithm for optimizations when minimizing in a region of incorrect curvature has been improved.

- The initial guess for AM1 and PM6 has been improved.

- More analysis of input ONIOM and MM parameters with respect to secondary structure is now done (by default for systems with <10,000 atoms when secondary structure information is available). The net MM charges on residues and average distances between residues are reported.

- Various performance improvements, including ones for larger numbers of SMP processors and for SCF frequency calculations.

Bug Fixes and Minor Changes between Gaussian 09 Revision A.02 and A.01:

- The logic for handling extra negative eigenvalues of the Hessian during minimizations has been improved.

- The combination of DFT and General SCF, automatically turned on if DFT is requested along with **Int=DKHSO**, does not work and is now rejected by the route generator.

- ONIOM input is now checked for divalent link atoms. The position of these atoms is ill-defined unless the distance scale factors are set to 1, and the model is usually poor if the scale factor is forced to be 1. Since this input is normally an error, it is now rejected by Link 101. IOp(1/132) can be used to force acceptance of this input, but this is strongly discouraged.

- Semi-direct integral transformation is the default. This code parallelizes better than the fully direct or in-core algorithms and is similar in speed on a single processor.

- A bug which caused **ONIOM=InputFiles** to fail when PDB secondary structure information was included in the input has been fixed.

Changes in Usage and Defaults between Gaussian 09 and Gaussian 03

- There are many changes in the PCM algorithms:

  - ❖ The default surface integration is new and gives continuous potential energy surfaces. It is strongly recommended for all new studies. The route option **SCRF=G03Defaults** restores most of the defaults to those in G03, but should be used only for comparison with previous calculations done using G03.

  - ❖ When using the default IEFPCM solvation method or **SCRF=CPCM**, Gaussian 03 computed and reported non-electrostatic contributions to the solvation energy but did not include these in the energies and they were not included in the energies used for geometry optimizations, frequencies, etc. By default Gaussian 09 does not compute these values at all.

  - ❖ The new SMD solvation model is recommended for absolute solvation energies and other properties for which the non-electrostatic solvation terms are significant. When **SCRF=SMD** is specified, the SMD non-electrostatic terms are included in

the basic energies (the SCF energy reported in the "SCF Done" line, correlated energies, etc.) and are included in the geometry optimization and frequency calculations. The non-electrostatic energy is also reported separately.

❖ Absolute solvation energies should be computed by doing a gas-phase optimization and frequency calculation on the system, followed by the same calculations with **SCRF=SMD** or **SCRF=(SMD, Solvent=…)**.

❖ The **SCFVac** PCM input option has been removed. If preliminary gas-phase energy is desired, do this in a separate job step before the solvated calculation.

♦ MP and CC calculations now default to a partial transformation (**Tran=IABC**). This is faster on most systems, especially when several processors are used. A full transformation can be requested using **Tran=Full**.

♦ The default SCF convergence is 10^8 on the density for all calculations, including single points.

♦ The physical constants used by default are those from the 2006 CODATA tables; those used in Gaussian 03 can be requested via **Constants=1998**.

♦ AM1, PM3, and PM3MM by default use the new semi-empirical code, which has proper analytic first and second derivatives but which gives slightly different total energies because it computes the overlap integrals via 6-Gaussian expansions rather than over Slater functions. **AM1=Old** and **Use=L402** both request use of the old (MOPAC 6) code, through the regular links or through link 402, respectively. The new code is strongly recommended except when comparison with results from Gaussian 03 is required.

♦ **Stable=Opt** defaults to the usual (L502) SCF procedure for the initial SCF but then uses **SCF=QC** for additional SCF calculations, if they are required.